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A Framework for the Integration of Green and Sustainable Chemistry into the Undergraduate Curriculum: Greening Our Practice with Scientific and Engineering Practices

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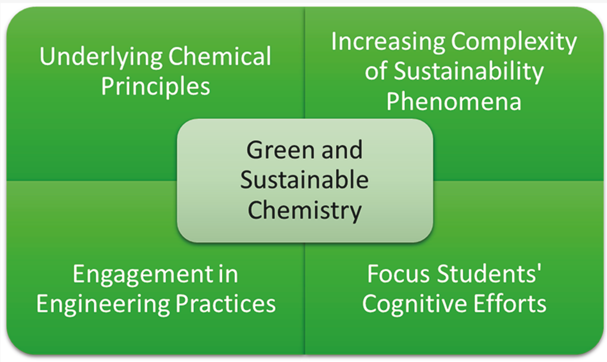
ABSTRACT: Green and sustainable chemistry (GSC) will become ever more central to the study of chemistry. This is demonstrated by commitments from the American Chemical Society, particularly the Committee on Professional Training and the Green Chemistry Institute, and the United Nations (UN Sustainable Development Goals), which underscore the urgent need for a paradigm shift in chemistry and chemistry education. Engagement in green chemistry education can provide students with connections between the chemistry they learn in the course and the environmental and human health consequences of chemistry in the world around them. The purpose of this position paper is to (a) reframe GSC as a decision-making activity, (b) briefly introduce theoretical principles for instructional design and assessment of student learning, and (c) describe a framework for the implementation of Green and Sustainable Chemistry that emerged from our designs of case studies using these theoretical principles. This framework includes four key design principles: (1) underlying chemical phenomena should be central to sustainable issues studied, (2) scaffold complexity over time, (3) students use engineering practices to support decision making, and (4) manage student cognitive load by deliberate use of analytic tools. Finally, we briefly discuss three case studies that were developed by using these principles as examples of this approach.



KEYWORDS: *First-Year Undergraduate/General, Second-Year Undergraduate, Upper-Division Undergraduate, Curriculum, Problem Solving/Decision Making, Green Chemistry, Learning Theories, Engineering Practices*

■ INTRODUCTION

Green and sustainable chemistry (GSC) has become essential to the study of chemistry, as demonstrated by commitments from the American Chemical Society's Green Chemistry Institute as well as international policy goals such the United Nations' Sustainable Development Goals (UN SDGs). These efforts underscore the urgent need for a paradigm shift in chemistry and chemistry education.[1] The call for green chemistry as a prominent feature in the training of future chemists and as a critical component in learning chemistry for all citizens has been growing for the past 20 years. For example, the American Chemical Society guidelines for undergraduate chemistry programs suggest that green and sustainable chemistry case studies be incorporated into curricula.[2] Since the initial proposal of the 12 Principles of Green Chemistry (GCPs),[3] educators have developed laboratory activities,[4−9] curricular materials,[10−13] and curricula[6,10,14−16] to address the pressing need for a green and/or sustainability focus in chemistry education. A 2012 review of the incorporation of green chemistry in higher education noted that, at the time, most primary green chemistry literature was in the realm of organic synthesis, leading to an emphasis in the organic chemistry curriculum.[17] However, in that 2012 review it was often noted that information about green and sustainable chemistry was presented in textbooks as "side bars and vignettes",[11,12] and at the time there were few assessments featuring GSC, which inadvertently communicated a lack of importance of GSC.[18,19]

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Table 1. Three Dimensions of Learning Adapted from the Framework for K-12 Science Education[62]

Dimension	Definition	Components
Core Ideas	Ideas with broad explanatory power that underpin a discipline and can be used to model, predict, or explain phenomena	Electrostatic and bonding interactions
		Atomic/molecular structure and properties
		Energy
		Change and stability in chemical systems
Crosscutting Concepts	Lenses to view phenomena and make connections that transcend disciplinary boundaries	Patterns
		Cause and effect
		Scale, proportion, and quantity
		Systems and system models
		Energy and matter
		Structure and function
		Stability and change
Science and Engineering Practices	Disaggregated components of inquiry and design that scientists and engineers perform; how we want students to demonstrate their knowledge	Asking questions (scientists) and defining problems (engineers)
		Developing and using models
		Planning and carrying out experiments
		Analyzing and interpreting data
		Using mathematical and computational thinking
		Constructing explanations (scientists) and designing solutions (engineers)
		Engaging in argument from evidence
		Obtaining, evaluating, and communicating information

By treating green chemistry as a set of topics[20] with no underlying core connections, curricular materials tend not to align with theories about the development of expertise,[19,21] which further compounds the fragmentary nature of student understanding of the discipline of chemistry. In our view, the 12 Principles of Green Chemistry are more appropriate for use by their intended audience, industrial process chemists with expertise and experience, rather than use by novice chemistry students. Expert chemists who have a wealth of experience to draw upon will be able to make those connections between molecular behavior and optimizing the process. Students are still building these connections from experience. For example, those who may have never experienced the less environmentally benign version of a "greener" process or reagent (*i.e.*, a chromium oxidation versus a "greener" oxidation), there is a considerable amount of prior chemistry knowledge that is required before their benefits can be appreciated.

In addition to the original work on the principles of green chemistry, more recent initiatives[22] to incorporate green chemistry into curricula have focused on overarching sustainability goals set by institutions such as the United Nations.[23] These efforts may also be increasingly coupled with a cocommitment to Systems Thinking[13,24−30] often discussed as a set of values about teaching science in the context of environmental and human systems[22,24,25] and, less frequently, as a set of performances to be embedded into curricular materials.[26,31−33] A popular approach for thinking in systems is the construction and use of systems diagrams.[34,35] Others have suggested performances of what a systems thinker should do, such as recognizing that the chemistry is embedded in a system rather than a collection of parts and examining relationships between parts of a system and how they lead to system behaviors.[29,31,32] Since this curriculum design project has begun, researchers have identified systems thinking skills for the undergraduate curriculum, although these tasks require explicit prompting to engage students at scalar levels below the macroscopic.[36,37]

While these initiatives represent big-picture ideals and are aligned with the core competencies proposed by MacKellar et al.,[38] less is known about how to enact these ideas within a curriculum and collect evidence from assessment tasks about what students know and can do with their green chemistry knowledge.[2,39,40] Sustainability and Systems Thinking are often shown as macroscopic level phenomena, as they involve observable and measurable problems in the real world, yet little is known about how to effectively connect the molecular-level basis of chemical phenomena to these large-scale systems. Although examples of prompting students with big-picture Earth systems and sustainability are present in fields such as Earth Science education,[22,41−47] in 2019 the few examples in chemistry education motivated us to create tasks to help students connect these systems to chemistry ideas in ways that support student use of scientific and engineering practices and disciplinary core ideas.[48,49] Furthermore, large-scale Systems Thinking representations and performances are reflective of expert behavior, requiring a specific focus on the connectivity of existing chemistry knowledge to provide a coherent understanding of the sustainability phenomena of interest.

In our view, it is important that chemistry educators understand that such expert-like behaviors are unlikely to develop in tandem with learning chemical principles needed to understand the phenomena since these expert-like behaviors are likely to be highly cognitively demanding. That being said, engagement in green chemistry education can provide students with connections between the chemistry they learn in the course and the environmental and human health consequences of chemistry in the world around them. Our proposed approach is that green and sustainable chemistry (GSC) can be considered as a set of decisions that one can make *using their chemistry knowledge* to help address these real-world issues. We propose that successful integration of GSC into the curriculum requires a consideration of how people learn and an understanding of how to use this knowledge to design curricular materials to support learning.[50−53] Thus, we outline

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an approach that leverages the *Framework for K-12 Science Education*[54] to incorporate GSC into the undergraduate chemistry curriculum; this approach frames "doing green chemistry" as the opportunity for students to engage in the engineering practices of defining problems and designing/evaluating solutions using their chemistry knowledge to make decisions. We also briefly discuss theory- and evidence-based approaches to curriculum design and student assessment. Finally, we conclude this paper with discussion and examples of four key design principles: (1) underlying chemical phenomena should be central to sustainable issues studied, (2) scaffold complexity over time, (3) students use engineering practices to support decision making, and (4) manage student cognitive load by deliberate use of analytic tools. These design principles were used to develop and enact the curricular architecture of the GSC case studies.

Theoretical Perspectives on Learning

This position is that green and sustainable chemistry be incorporated into curricular materials as guidelines for decision making rather than ideas that students should learn. In this way the instructional focus switches from *how shall I teach* to *what performances would convince me that the students are using GSC ideas to make decisions*: the emphasis moves from *teaching* to *learning.* So, our instructional design strategy has placed emphasis on scaffolding students with the appropriate materials and knowledge needed to engage in decision-making through the lens of green and sustainable chemistry. That is, we intentionally design activities that support student recall of appropriate chemical principles that underlie the system being investigated or discussed. Then, with the appropriate chemical knowledge students can apply green and sustainable decision making to the system under consideration.[55,56] That is, we position learning green and sustainable chemistry as an opportunity for students to *use* their knowledge while defining problems and designing and evaluating solutions to those problems.

This approach is closely aligned with what has come to be known as three-dimensional learning (3DL).[18,57,58] Originally put forth in a consensus study from the National Academies of Science in *A Framework for K-12 Science Education*, this evidence-based and theory-backed vision for science education has been increasingly accepted and implemented in higher education.[59−61] This adaptation for higher education chemistry is illustrated in Table 1.

One of our coauthors (MMC) has been central in the development of a set of chemistry Core Ideas, which are explanatory for a wide range of phenomena and can be used in increasingly sophisticated ways. These Core Ideas differ from other approaches such as defining "Anchoring Concepts"[63,64,64−66] in that they are not discrete topics (such as kinetics or atomic structure) but rather the underlying ideas that can support understanding of a range of topics. For example, the topic of solubility relies on the core ideas of structure−property relationships, forces and interactions, and energy. Our ultimate goal is to help students develop connected and useful knowledge, and using core ideas helps students connect seemingly disparate topics. If students learn topics in isolation, their knowledge structures are often fragmented and not useful in new situations.[67] Knowledge structured around and connected to the Core Ideas can be used in new situations, such as to guide green and sustainable decision-making.

Cross-Cutting Concepts (CCCs) can be thought of as tools or lenses through which to focus on a particular aspect of phenomena both within and across disciplines.[68] They can be thought of as rules of the game or epistemic heuristics that are often implicit in instruction, but designing activities that scaffold such ways of thinking allows students to access and use them across different phenomena. In previous work, a focus on Cause-and-Effect (Mechanism and Explanation) has been used to understand how students develop mechanistic reasoning,[69−72] which has been shown to lead to more equitable outcomes.[73] However, there are many CCCs that are particularly relevant to GSC, such as exploring the Flows, Cycles, and Conservation of Energy and Matter or the complexity within Systems and System Models.

Scientific and engineering practices are the things that scientists and engineers do. They include practices such as designing and carrying out experiments and constructing arguments from evidence, as shown in Table 1. Explicitly building these practices into instruction allows us to look for evidence that students can use them (rather than trying to characterize more amorphous outcomes such as "critical thinking" or "higher order thinking").

3DL requires that core ideas, crosscutting concepts, and scientific and engineering practices be inextricably intertwined. That is, learning and assessment tasks should include all three dimensions rather than focusing on content alone. By explicitly defining the types of learning that we are trying to support in our students, we allow us to design assessment tasks that have the potential to elicit evidence of such learning.

There is now an increasing body of work supporting the use of 3DL in higher education.[58−62] As discussed below, an emphasis on engagement in the engineering practices of defining problems and designing and evaluating solutions was prioritized; these engineering practices serve as the basis of tasks in which students will use their knowledge of the core ideas of chemistry to engage in green decision-making.

Engineering Practices

As noted above, our approach is that the nature of making decisions can be structured within a three-dimensional learning (3DL) framework that emphasizes student engagement in engineering practices. By framing GSC as such, students are poised to incorporate the core concepts of chemistry in pursuit of an understanding of the underlying mechanism causing the sustainability issue under study. Furthermore, by situating the GSC in the context of real-world problems, students can engage in engineering practices and see the sustainability problem through the lens of various impacted groups or people who have a vested interest, *i.e.*, the stakeholders.

Specifically, this decision-making scaffold was designed using the engineering practices of defining problems and designing and evaluating solutions, as described by the *Framework for K-12 Science Education*.[54] As students define the chemical and environmental problem at hand, they are encouraged to think more deeply about why it is a problem and be able to define the criteria and constraints of interest to the groups of stakeholders impacted by the problem. With these criteria in mind, students can more easily be prompted to systematically evaluate the acceptability of the proposed solutions, engineer their own solution to the problem, and balance trade-offs between competing perspectives and solutions to the problem at hand.[74] Although engineering practices are rarely incorporated into chemistry curricula in higher education,[75] we

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envision that they can act as the vehicle that drives the decision-making involved in real-world chemistry problems. By using engineering practices as part of the framework for instructional design, we can target specific performances that will elicit robust evidence of the desired learning performances. We believe that engagement in these practices can elicit more sophisticated, expert-level decision-making over time and will better prepare students for a career in STEM and to be a STEM literate citizen.

■ METHODOLOGY

Design-Based Research

To determine whether a particular set of materials and learning conditions can support students to use their knowledge in these relatively sophisticated ways, the research method of design-based educational experiments was adopted to allow for naturalistic learning conditions.[50,76] One approach to this type of research is a design-based research cycle, as shown in Figure 1.

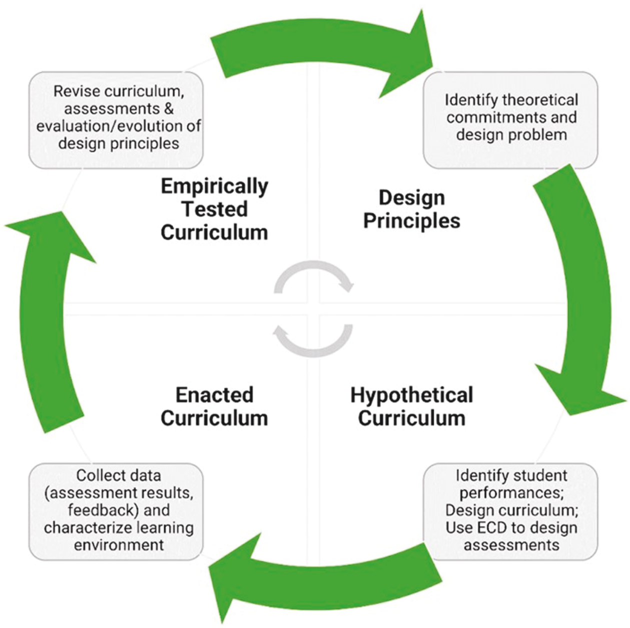

Figure 1. Design-based research cycle tailored to the development of this green chemistry curriculum.[77]

This research cycle starts in the upper-right quadrant, specifying the design principles that will guide and focus the curricular materials. This is accomplished with the identification of theoretical commitments (*e.g.,* green and sustainable chemistry, three-dimensional learning, with emphasis on the engineering practices) and a narrow definition of the design problem, namely, the search for evidence that students can use their core chemistry content knowledge to explain and make decisions about green and sustainable chemistry phenomena. From those design principles, a hypothetical curriculum can be generated through backward design.[78]

To develop the kinds of formative assessment tasks that will elicit strong evidence about student learning, the research team has embedded a modified evidence-centered design (m-ECD) process for generation of specific tasks, as described below. By identifying key student learning performances that serve as the goals or claims, course designers can generate curricular activities to engage students and design specific assessments to anchor these activities. Then the students' responses can be used as evidence as to whether the students have met the goals set by the designer. Once the curriculum is enacted, collection of multiple strands of data (such as student response artifacts, interview and surveys for student and instructor feedback, and observations of the student engagement) can be used to characterize the learning environment and refine activities and assessments. While this design-based research cycle highlights the approach to curriculum development, enactment, evaluation, and refinement, this project has embedded a modified evidence-centered design process (as detailed below) to serve as the primary method of characterizing the impact of our intended curriculum on students. In this article, the focus is on the first two quadrants of the Design-Based Research cycle in which the design framework for green and sustainable chemistry is defined and the architecture of the curriculum is outlined based on the commitments to four key design principles.

Evidence-Centered Design

This approach to designing assessment tasks fits into the larger cycle of design-based research[50,79] described above. The curriculum designed from this process uses the pedagogical technique of scaffolding student ideas across tasks to support reasoning. To accomplish this in a coherent manner, a modified evidence-centered design (m-ECD) process was employed.[80,81] ECD (Figure 2) is based on the idea that assessment of student learning requires the construction of an evidence-based argument, where the evidence is the product that the student produces.[67] ECD requires that the developer think through the specific claims about student knowledge, the evidence one would accept to demonstrate the claim about student knowledge, and then design the student-facing task that elicits this particular evidence.

While this process is not appropriate for every task or assessment prompt within the curriculum, this structured unpacking process helps us to think through prompts that will be used to elicit evidence of what students know and can do. These assessment anchor points are chained together through the scaffolding process[82,83] that "builds up" to these tasks through the engagement with introductory, simpler tasks throughout the course of an activity or assessment and the strategic use of scaffolded tasks to structure student responses.

Design Framework for Green and Sustainable Chemistry

As noted in the introduction, many phenomena on the green and sustainable chemistry wish list include those of global importance, such as the UN SDGs, or a desire for students to be able to map out the intersecting systems of scientific enterprise, sociopolitical context, and the larger ecosystem.[34,36,37] These systems are many scalar levels above the atomic-molecular behavior and macroscopic indicators of a chemical reaction that chemists normally focus on in the undergraduate chemistry curriculum. One way of visualizing these systems at different scalar levels is in Figure 3, based on a figure from David Constable-Chichester from the American Chemical Society (ACS) Green Chemistry Institute (GCI), which outlines a series of system scales at various grain sizes from complex Earth systems down to the atomic/molecular-level. The descriptions of these system scalar levels have been edited to place an emphasis on the subatomic level that is necessary for reasoning about chemical phenomenon.[84−88] The lowest three scalar levels in this figure represent those that

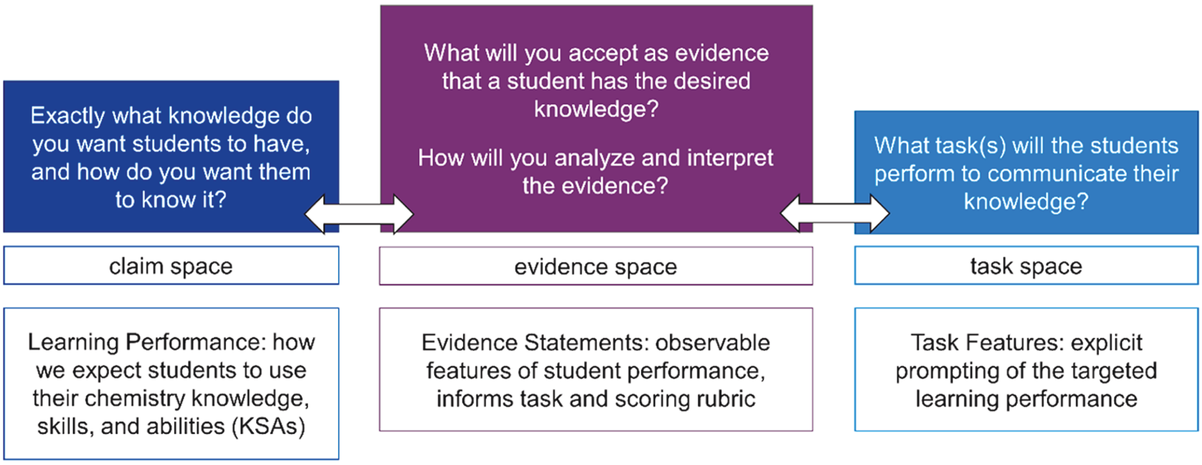

Figure 2. Modified Evidence-Centered Design (m-ECD) approach. Adapted from Mislevy and Haertel (ref 80). Copyright 2006 Wiley.

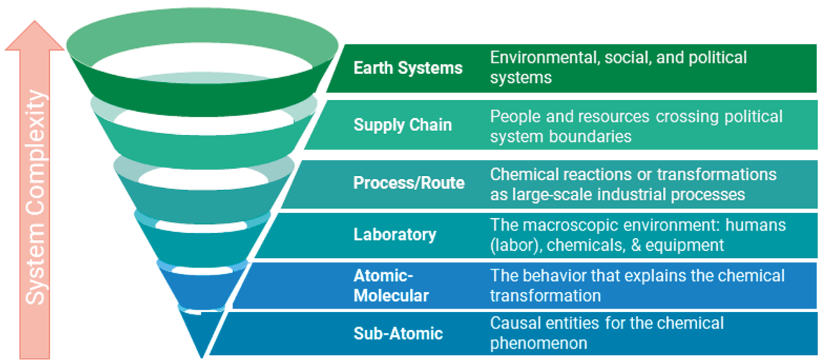

Figure 3. Series of system scales and their descriptions, showing increasing levels of system complexity. Adapted from personal communication with David Chichester-Constable at the ACS Green Chemistry Institute (ref 89). Copyright 2021 American Chemical Society.

are the focus of most current curricular offerings, and the upper three levels are critical system levels to consider when engaging in green and sustainable thinking. As noted in the original presentation, from a systems perspective, these levels increase in complexity as one moves from atomic-molecular systems to Earth systems.

Figure 3 also illustrates a fundamental tension in chemistry education. These three lowest levels (subatomic, atomic-molecular, and laboratory) comprise systems levels that are familiar to chemistry educators from the initial work of Johnstone,[90] who noted that chemistry students struggle to connect their budding conceptions of atomic/molecular behavior with symbolic representations and the macroscopic effects witnessed on the laboratory bench. This difficulty was most recently noted in Szozda et al.[36] Given that even these smaller more familiar scales of systems levels present real learning barriers for students, great care must be taken to help students connect the complexity of larger system presented to the underlying chemistry. In this project, our stepwise approach (as briefly described below) is intended to gradually increase the complexity of the phenomenon while also scaffolding the ways in which students are explicitly asked to make green(er) decisions based on their understanding of the chemistry underpinning these sustainability issues.

The remainder of this paper presents specific design principles for GSC curricular materials that have emerged from our work. This discussion briefly describes three examples of case studies, which will be described in greater detail and analyzed in future articles, which were designed using this set of design principles.

Design Principle #1: The Underlying Chemical Principles of Sustainability Phenomena Should Be Emphasized and Supported

The first design principle (abbreviated DP #1) to emerge was that a phenomenon should be selected to both support explanations at the level of the course in which the students are enrolled and foster green and sustainable decision-making. As previously noted, sustainability issues are often conceptualized on larger system scales, such as Earth systems (Figure 3), but in order to teach about complex phenomena and systems in a chemistry course, the chemical principles underlying the phenomenon at hand must have been previously learned—either in an earlier course, or in the course at hand. That is, each case study is not a vehicle for learning the basic principles, but rather, those chemical principles they have previously learned will be used in the context of green and sustainable chemical systems. For example, a focus on peptide bond formation in a case study was chosen because the students had previously been engaged in the lecture course in constructing mechanistic explanations of carbonyl chemistry; the students were expected to focus on using their extant mechanistic understanding in the context of evaluating the synthetic routes. However, it is almost certain that students will struggle with using their chemical knowledge in a new context. Indeed, the transfer of knowledge from one context to another is notoriously difficult. For this reason, it is important to scaffold

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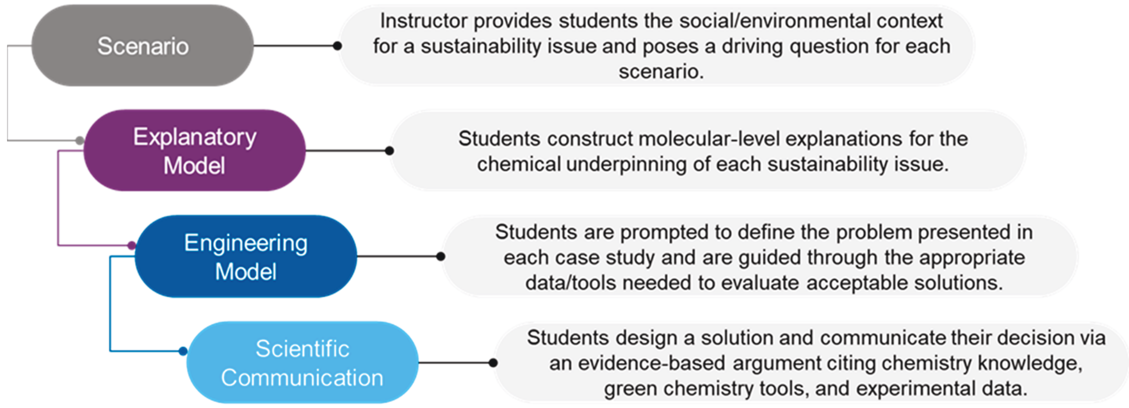

Figure 4. Enacted case study design architecture.

the introduction and use of existing knowledge by appropriate task design to help students recall the ideas they will be using in the new and certainly more complex context than the one in which they initially learned.

Design Principle #2: The Complexity of Sustainability Issues Addressed Should Be Increased over Time

The second design principle (abbreviated DP #2) emerges from the idea that most students will have had little prior exposure to life cycle and/or Systems Thinking. As described by its proponents,[26,34] performing a life cycle analysis (or thinking in systems) is an expert-like behavior. These performances may involve ideas, calculations, and visualizations that are mostly unfamiliar to novice students. Furthermore, making connections between (and constructing explanations of) the underlying chemistry and sustainability issues is not trivial. Therefore, the second design principle proposes that as students become more familiar with the tools and approaches of the GSC, then the system complexity can increase. For example, situating a case study at a particular system level can help develop the green and sustainable skillsets (such as applying green metrics to analyze the problem) and can be subsequently leveraged in a case study at a larger system level. Of course, this principle is determined by the experiences of the target student group: the starting point will depend on the familiarity of the students with GSC and their thinking about complex systems. Again, it is noted that if students are expected to learn both the chemical principles and the sustainability issues involved in GSC, the tasks will either become quickly overwhelming, or one of these aspects will be "short changed."

Design Principle #3: Engagement with Engineering Practices Can Support Decision-Making

Following our third design principle (abbreviated DP #3), the engineering practices of defining problems, designing solutions to problems, and evaluating potential solutions can be used to scaffold and guide students' decisions about GSC phenomena. As noted earlier, tasks that incorporate both chemical knowledge and GSC principles are complex and require students to assemble, connect, and use numerous disparate ideas and tools. Thus, tasks must be scaffolded to help students move through both chemical principles and decision-making activities in a productive manner. Specifically, this scaffolding is composed of prompts for a definition of the problem and an evaluation or design of a solution separately and iteratively, with intermediate prompts to push students to consider specific stakeholders and the criteria and constraints related to that set of stakeholders. In our experience, scaffolding of complex tasks is much more likely to elicit evidence that students are connecting and using their knowledge appropriately.[91,92] Lack of guidance to students tends to result in confusion and less productive responses that discuss surface level ideas such as descriptions rather than explanations about causal factors.[69]

Design Principle #4: Focus Students' Cognitive Efforts on the Important Ideas Rather than on Esoteric Tools and Metrics

The fourth design principle (hereby abbreviated as DP #4) focuses on what the curriculum developer would like students to take away from the overall task: that is, what do "we" want students to do with their knowledge? For most students, this project team believes that understanding chemistry and the use of evidence to make decisions about how to address system problems are most important. However, particularly as systems become more complex, there are specialized tools and metrics that are commonly used by experts that may obscure important ideas and desired learning outcomes. For example, if the goal of the task is for students to learn to calculate Eco-Scale[93] scores or other green chemistry metrics, then productive use of this tool should be a central focus. However, if the desired learning performance is to use Eco-Scale scores (or other specialized tools or calculations) as evidence to support decision-making, it may be better to provide these data and an explanation of what they mean, rather than requiring students to learn how to do it. In short, as the task becomes more complex, it becomes even more essential to focus on what was designated as the most important aspect of the task.

Case Study Design Architecture

Following the commitment to three-dimensional learning (3DL) and our guiding design principles, three multiweek case studies were designed that follow a common architecture (Figure 4) through which students engage in decision-making using green and sustainable chemistry.[94] In this approach, students were provided the necessary green and sustainable chemistry evidence and tools in conjunction with eliciting foundational chemistry core ideas to support students toward decision-making. Each case study starts with core chemistry knowledge that is used to explain molecular-level chemical phenomena and moves to scaffolded prompts aimed at engaging students in engineering practices to conceptualize the sustainability problem and evaluate acceptable solutions.

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The final activity of each case study asks students to decide how to best approach the problem, ideally by combining their understanding of the underlying chemistry with their analysis of the problem and potential solutions. Below, the first case study is used to exemplify the case study design architecture, as highlighted in Figure 4, followed by a brief overview of the scenario involved with our second and third case study activities.

A scenario is chosen that has societal relevance and one in which chemistry is a major contributor to the phenomenon of interest (DP #1). In this set of case studies, the provided scenarios started at the familiar laboratory bench scale and moved to larger systems scales, to slowly increase the system complexity as the students work towards the Earth Systems scale (DP #2). Starting at a familiar systems scale sets up students' expectations for the rest of the curriculum and models new performances on which they will build throughout the course. To illustrate this, a brief description of how this architecture applies to the first case study is provided below. Each "part" (the explanatory model or the engineering model) takes approximately a weekly 1 h meeting to complete.

The first case study uses green chemistry strategies (Figure 5) to support students as they construct mechanistic explanations of carbonyl chemistry highlighted by three similar synthetic pathways. This familiar context for students occurs at the laboratory system scale, and is framed similarly to the laboratory projects they have experienced in general chemistry and/or in the laboratory portion of their organic chemistry laboratory course.[94] In the explanatory model (first part of each case study), students are prompted to construct explanations for portions of the underlying chemistry (*i.e.*, nucleophilic attack on a carbonyl carbon) and make connections to the sustainability issue at hand (DP #1) so that they can evaluate synthetic pathways embedded in the problem. In the engineering model (second part of each case study), students are asked to use their understanding of the chemical phenomenon to define the problem, as framed by the scenario. Students are scaffolded to engage in the engineering practice of evaluating solutions (DP #3) to evaluate the three possible reaction schemes, decide on which of the three best satisfies the stakeholders (the environmental team, the synthesis team, and the accounting team), and support their decision with appropriate reasoning. By prompting students to consider different stakeholders,criteria, and constraints associated with the problem (*i.e.*, cost, percent yield, byproducts, solvent waste), the aim is to productively support students to use their chemical knowledge and data/tools to make decisions pertinent to the scenario (DP #4). Lastly, in scientific communication (final part of each case study), students focus on using data, tools, evidence, and scientific knowledge to evaluate acceptable solutions (DP #3) and communicate their final decision to nonscientific audiences. These choices are intentional: within this well-scaffolded case study, students are prompted to *use* their existing knowledge and are not provided with superfluous details.

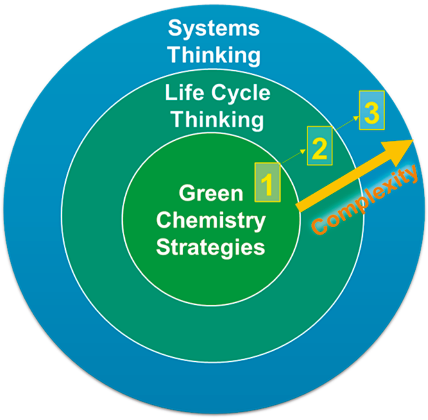

Figure 5. Green chemistry reasoning strategies utilized at increasing levels of system complexity. Adapted from Ginzburg et al. (ref 27). Copyright 2019 American Chemical Society and Division of Chemical Education, Inc.

The second case study extends to the Process/Route scalar level (Figure 3) to introduce aspects of life cycle thinking (Figure 5). This case study invokes the core ideas of change and stability and electrostatic interactions related to polymerization reactions and recycling methods, and the scenario is framed so that students may evaluate solutions to the problem of plastic pollution at two different time points in the life cycle. The first point in this qualitative life cycle analysis is the sourcing of monomers and the green metrics associated with the synthetic route for each monomer ("beginning-of-life"). The second point in the life cycle to be evaluated is the methods of recycling, biodegradation, and compostability of polymerized materialized materials using the data provided ("end-of-life"). Again, students begin by developing a mechanistic explanation of the underlying chemistry by using knowledge they have previously learned. Then they are asked to define the problem at both time points, which includes developing criteria for acceptable solutions and determining what constraints there might be on the solutions. Finally, they use the data provided and evaluate their potential solutions to justify which solution to support in a policy paper.

The final case study presents a sustainability study that encompasses a scenario at the Earth systems scale (Figure 3). This scale is more complex and, thus, the scenario is less well-defined than the previous two case studies. Students use the core ideas bonding and interactions and structure property relationships to understand the properties of a class of molecules: perfluoroalkylated substances (PFAS). Their task is to define the environmental problem by first recognizing how both the desirable and the undesirable properties of PFAS are explained by their molecular structure. That is, why are PFAS so useful in so many ways but so hard to remove from the environment? Instead of directly engaging students in the construction of a system diagram (as might be done with a Systems Thinking task), students were asked to use a provided system diagram (based on data and government policy documents) in conjunction with the chemical properties to design a solution to the PFAS pollution problem in a local area.

■ DISCUSSION

In these case studies, chemical principles were chosen that students have already recently seen in an organic chemistry class—such as nucleophilic attack at a carbonyl carbon. Alternatively, students were scaffolded toward chemistry that they may have learned in an earlier course and have not used recently, such as the mechanisms by which solutes dissolve (or do not dissolve) in solvents. By carefully constraining the underlying chemical principles, the goal was to focus students' attention on how that chemistry contributes to the sustainability issues that emerge from the use of different

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synthetic routes, at different time points in an overall life cycle, and at the intersection of multiple systems. Our first design principle guided us toward phenomena that have sustainability implications that also rely on chemical principles that students can use to explain the problem.

Our second design principle guided us to start with a smaller scale and move toward a more complex, interconnected system in a sequential manner. This approach follows the logic illustrated above in Figure 5, adapted from experts of green chemistry, on the types of reasoning about sustainability that can be paired with our focus on using mechanistic understanding of the underlying chemistry to help make evidence-based decisions. Figure 5 demonstrates that green chemistry strategies are theorized as a core competency that can be applied throughout the life cycle of a chemical process and how these considerations may intersect with, and therefore require, thinking about how systems intersect. The yellow boxes are intended to map out the three case studies for this project, and the orange arrow demonstrates that the sustainability issues in these case studies increase in system complexity. This sequential approach allows us to carefully scaffold the chemical knowledge and resources required to approach each problem across this set of case studies.

Within each case study, we also scaffolded students toward engagement in engineering practices (our third design principle) designed to have them define the problem in each scenario before designing and evaluating solutions to the problem. Upon testing early iterations of this curriculum, it was found that student use of green chemistry tools and metrics was highly unproductive, as it seemed to distract from engaging in our engineering practices of interest. For example, instead of asking students to calculate an Eco-Scale score from a set of decontextualized procedures and scientific data, the intent was to lessen student cognitive burden by providing preassembled data sets for various green and sustainable chemistry metrics (our fourth design principle).[33] With these data presented to them, students were tasked with analyzing information (a scientific practice) to support their argument for their decision (another scientific practice) as to which solution to follow for either of the case studies. As a result, the finding was a balance between engagement in engineering practices and productive reasoning with green and sustainable chemistry data and tools as students worked through their decision-making process.

■ CONCLUSIONS AND FUTURE WORK

This section offers a summary of our work and its implications for further research and adoption by green chemistry educators. The overarching goal of this manuscript was to outline the first two quadrants of the Design-Based Research cycle (Figure 1) through which four key design principles were developed that guided our development of a green and sustainable chemistry curriculum via three multiweek case study activities. For students to engage in constructing explanations *and* scaffolded decision-making, they must have some prior understanding of atomic-molecular behavior and a tailored amount of information to manage cognitive load for a case study that extends over a 3- or 4-week timeframe. Any curriculum in which GSC is introduced should build complexity over time, scaffold decision-making with engineering practices, and avoid introducing skills and activities that are not strictly necessary.

Following the commitment to the modified evidence-centered design (m-ECD) process, expectations of student performance were defined during case study activities to be (1) construct explanations about the chemical underpinnings of each sustainability phenomena, (2) define the scope of the problem posed in each case study, and (3) coordinate chemical knowledge and data to design/evaluate solutions to sustainability issues. In enacting this curriculum, the two main types of student response data were weekly formative assessment tasks (the explanatory and engineering model components of the design architecture) and summative reports (the scientific communication component of the design architecture), in which students communicate their solution to the problem posed in each case study. Ongoing efforts by our research team are focused on analyzing the student response data from these tasks and characterizing student engagement in engineering practices at each step along the way. Future manuscripts stemming from this work will elaborate on how the data analysis related to each case study informs the task refinement process as iterative changes were made to the curriculum to better support students in achieving the targeted performance expectations.

While the products of design-based research are highly contextual, a robust instructional design may be adaptable to other institutional contexts. We recognize that the organization, performance selection, and pacing of our design reflects affordances (such as students being enrolled in transformed curricula for general and organic chemistry that support the development of core chemistry ideas) and limitations, for example, the time available and the course context (lecture, lab, workshop). The content and flow of the curriculum materials described here may not transfer directly to another institutional context, but the *framework of how to approach the design, implementation, and evaluation of these curricular materials* is broadly applicable and is, we believe, a potentially valuable approach for how green and sustainable chemistry phenomena might be incorporated into all chemistry curricula.

■ LIMITATIONS

We acknowledge that there are several limitations to this approach. For example, our reliance on engineering practices to structure the green and sustainable chemistry aspect is a "good fit" for the transformed courses, in which the case studies are included. We have found that students in more traditional courses, which do not emphasize the other scientific practices such as construction of models, explanations, and arguments are less likely to be able to construct explanations and engage in decision making. However, the four design principles that we describe should be applicable to a wide range of course structures and situations, provided that the learning and assessment goals are clearly specified.

Our design examples also reflect the constraints of a large-enrollment course that serves a variety of STEM majors (not just chemistry majors). In this course the case studies were used in a one hour session once per week for 12 weeks. This meant that it was not possible to fully explore all aspects of Systems Thinking or GSC. In addition, the course was taught by graduate teaching assistants, who may not have had deep knowledge of GSC themselves. However, as we report in a future paper, these students were still able to complete the case studies and make evidence-based decisions about the problem at hand.

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Notes

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